Indian J. Phys. **76A** (6), 553-555 (2002)

IJP
— an international journal

Monte Carlo calculation of electron transport in InSb

P S Mallick*
Department of Electronics and Communication Engineering,
National Institute of Science and Technology
Palur Hills, Berhumpur-761 008, Orissa, India

and

D Mukhopadhyay
Device Modeling Laboratory,
Department of Electronics and Telecommunication Engineering
Jadavpur University Kolkata 700 032, India

E-mail psmallick@yahoo.com

Received 29 May 2002 accepted 9 August 2002

Abstract The velocity field characteristics of InSb have been obtained at 77K by the Monte Carlo simulation technique. The results agree with the experimental data and also with those obtained by using the displaced Maxwellian distribution function. The effects of the various simulation parameters as well as that of the ionized impurity concentration on the mobility values for InSb have been discussed and results presented.

Keywords Compound semiconductor, Monte Carlo simulation, mobility- field characteristics

PACS Nos. 61.43.Bn, 72.20.Dp,

1. Introduction

Indium antimonide (InSb) is a widely used material for solid state electronic devices. Electron mobility in this material has been obtained using the displaced Maxwellian distribution function under different physical conditions [1-4]. The analytical methods for obtaining the conduction properties in semiconductors is beset with many complications. Various approximations not all of which can be justified, have to be used to obviate these difficulties under high field conditions. The Monte Carlo (MC) technique provides a better and more rigorous solution in such a situation. The MC simulation method has become a standard numerical technique for theoretical studies of the electron mobility as well as transport properties of hot carriers in semiconductors. This technique has been used by many workers to obtain the velocity-field characteristics of various [5] compound semiconductor. The present work gives a more detailed study incorporating almost all the important scatterings like the ionised impurity scattering, polar optic phonon scattering, acoustic phonon scattering, piezoelectric scattering as well as the screening effect. Here, the electric field is considered ($E \leq 1$kV/cm) and the magnetic field is ignored, since significant changes of electron mobility can occur only when the electric field intensity is higher or of the order of 1 kV/cm [6].

*Corresponding Author

2. Band structure and dispersion relation

The simple expression relating the energy E above the minima of the conduction band and the wave vector of the carrier $\boldsymbol{k}$ is given by

$$E = \left(\hbar^2 k^2\right)/(2m^*), \tag{1}$$

m^* is the electron effective mass at the bottom of the conduction band. This expression known as the parabolic band approximation, neglects the effect of the bandgap.

We have assumed a simple nonparabolic band structure in our calculation such that the $\boldsymbol{E}-\boldsymbol{K}$ relationship is given by [7]

$$\gamma(E) = \left(\hbar^2 k^2\right)/(2m^*) = E(1+\alpha E), \tag{2}$$

where $\alpha = E_g^{-1}(1 - m^*/m)$ $\quad \dfrac{E_g \Delta}{3(E_g + 0.67\Delta)(E_g + \Delta)}$

and $\delta\gamma / \delta E = 1 + 2\alpha E$.

In the above approximation, the relations namely, (i) E as a function of k, (ii) k as a function of E, and (iii) $\delta\gamma / \delta E$ as a function of E are explicit and hence their incorporation in a Monte Carlo program is straightforward.

3. Scattering rates

The scatterings that have been considered here are scattering by ionized impurity atoms, by polar optical phonons and by acoustic phonons through deformation potential coupling and through piezoelectric interaction. Each of these collisions characterized by the scattering rate $S_i(\boldsymbol{k})$ which is the number of collisions of the ith type per unit time per unit volume in the $\boldsymbol{k}$ space, is given by

$$S_i(\boldsymbol{k}) = \left(\frac{V_c}{8\pi^3}\right)\int \frac{2\pi}{\hbar}|M(\boldsymbol{k},\boldsymbol{k}')|^2\,\delta(E_k - E_{k'})\,d\boldsymbol{k}', \quad (3)$$

where V_c is the crystal volume, $\boldsymbol{k}$ and $\boldsymbol{k}'$ are respectively the electron wave-vector before and after collision. $M_i(\boldsymbol{k}, \boldsymbol{k}')$ is the matrix element for ith scattering mechanism and can be written as

$$|M_i(\boldsymbol{k},\boldsymbol{k}')| = \left[A_i(|\boldsymbol{k} - \boldsymbol{k}'|)\right]^2 G(\boldsymbol{k},\boldsymbol{k}'), \quad (4)$$

$G(\boldsymbol{k},\boldsymbol{k}')$ is the overlap function, and A_i is the matrix element without the overlap function and is given for the different scattering mechanisms as [7],

$$A_{imp} = \left(Ze^2 / V_c\varepsilon\right)\left(|\boldsymbol{k} - \boldsymbol{k}'|^2 + \lambda^2\right)^{-1},$$

$$A_{ac} = E_1\left(\hbar / 2V_c\rho\omega_q\right)^{1/2}(e_q.q)\,F(q,\lambda),$$

$$A_{pz} = \left(eh_{pz} / \varepsilon\right)\left(\hbar / 2V_c\rho\omega_q\right)^{1/2} F(q,\lambda),$$

$$A_{pop} = \left(e/q\right)\left(k_\infty^{-1} - k_0^{-1}\right)\left(\hbar\omega_1 / 2V_c\varepsilon_0\right)^{1/2} F(q,\lambda),$$

where $F(q,\lambda) = S_i(q,\lambda)\left(n_q + \tfrac{1}{2} \pm \tfrac{1}{2}\right)$,

λ is the Debye screening length, E1 is the acoustic phonon deformation potential coupling constant, e_q is the unit lattice vector, h_{pz} is the piezoelectric constant, ω_1 is the longitudinal polar optical phonon frequency, $q = |\boldsymbol{k} - \boldsymbol{k}'|$ and Z is the degree of ionization of the impurity atoms, assumed unity.

$S_i(q,\lambda) = q^2 / \left(q^2 + \lambda^{-2}\right)$ is the screening factor.

Substituting the appropriate matrix elements and carrying out the integration in (3), the rates for the different scattering processes and hence the total scattering rates are evaluated

4. Results and discussion

We have followed the procedure of Fawcett *et al* for Monte Carlo simulation[5]. The program for Monte Carlo simulation is written in C and the material parameters used are

$m^*/m_0 = 0.0146$, $\kappa_0 = 17.88$, $\kappa_\alpha = 15.68$, $\rho = 5.77$ gm. cm^{-3}

$\theta_D = 292$ K, $K_m^2 = 0.027$, $Eg_0 = 0.24$ eV, $\Delta = 0.9$, E1 = 30 eV

Formulations for computation of different band properties, such as overlap integral, $\delta\gamma / \delta E$ *etc.* are included in the program. Also included are scattering rate computation routines for various scattering processes. The simulation is found to converge after between 50 and 100 thousand real scatterings depending upon the applied electric field and ionized impurity concentration. The calculated results agree satisfactorily with the available experimental data and with the calculations based on analytical techniques like those using displaced Maxwellian distribution function. As an example, we note that for InSb at 77K, the mobility obtained by Monte Carlo simulation is 46.47 $m^2 V^{-1} S^{-1}$ while that obtained by using the displaced Maxwell distribution function is 45 $m^2 V^{-1} S^{-1}$ at a field of 50 V/cm [4] and the experimental value of mobility at this field is 50 $m^2 V^{-1} S^{-1}$ [1]

In Figure 1, we have plotted the variation of electron mobility with the applied electric field in InSb for zero ionized impurity concentration and also for ionised impurity concentrations of 1e14 and 5e14 cm^{-3}. It is found that the mobility decreases monotonically with the applied electric field for all these curves. At high enough fields above 1kV/cm, the mobility values are insensitive to the ionised impurity concentration indicating the gradually diminishing contribution of ionised impurity scatterings at high fields. The field dependence of mobility also

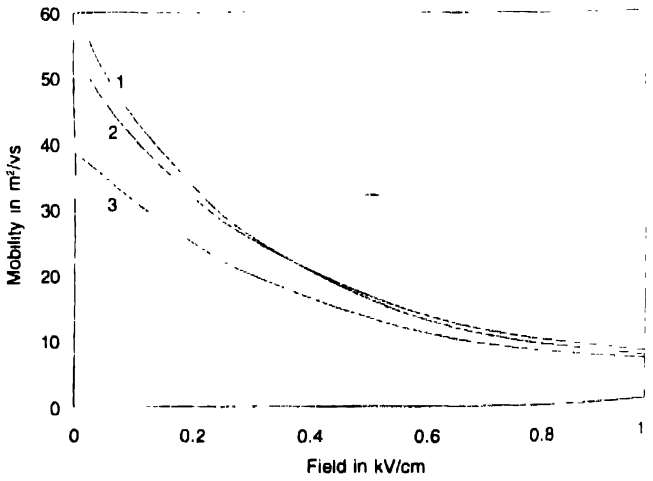

Figure 1. Variation of electron mobility with applied electric field in InSb at 77K for different ionized concentrations. (1) Ni = 0, (2) Ni = 1e14 and (3) Ni = 5e14 cm^{-3}.

shows sharper variation in samples with lower impurity concentrations.

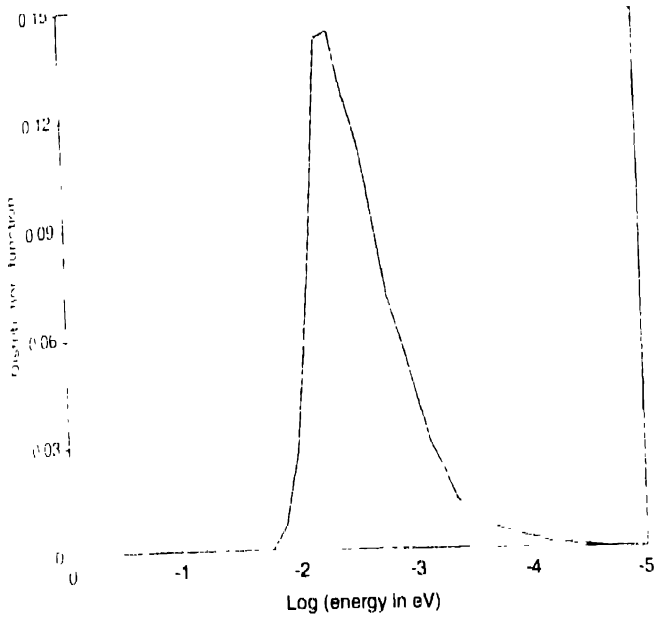

Figure 2. The distribution function in InSb at 77K for an applied electric field of 100 Vcm^{-1} and for zero ionized impurity concentration

The distribution function of the electrons has also been obtained from the results of these computations. For this purpose, the entire k space is subdivided into a large number of cells and the time the electron spends in a particular cell of the k space is logged and this value is normalized by the total time. This gives the probability of the electron being in that cell, and hence the energy distribution function. The normalized distribution function thus obtained is shown in Figure 2 for InSb at 77K for an applied electric field of 100 V/cm and zero ionized impurity concentration.

5. Conclusion

We have followed the technique used by Fawcett, Boardman and Swain [5] for simulation. It has been found that the result varies with "Rees Parameter" The concept of "missed collision" has also been included here.

References

[1] M Glicksman and V Jr Hiembothem *Phys Rev* **129** 1572 (1963)

[2] D Mukhopadhyay and B R Nag *Indian J Pure Appl Phys* **7** 616 (1969)

[3] E De Alba and J Warman *J Phys Chem of Solids* **29** 69 (1968)

[4] T Y Stokoe and J F Cornwell *Phys Stat Solidi* **B49**, 651 (1972)

[5] W Fawcett, A D Boardman and S Swain *J Phys Chem Solids* **31** 1963 (1970)

[6] EA Mendes, EWS Caetano and V N Freire *Appl. Phys Lett* **70** 1879 (1997)

[7] B R Nag *Electron Transport in Compound Semiconductors* (Solid State Science Series) (Berlin Springer-Verlag) (1980)